

The Origin of Diamond-Hexagonal Silicon

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Using the Berkeley Atomic Resolution microscope, researchers have been able to obtain direct confirmation for their model of the origin of diamond-hexagonal silicon, a recently discovered structural modification of silicon. This breakthrough proves that shear stresses, rather than hydrostatic pressure, are the cause of the observed structural modification.

Background - Although at high pressures silicon is found in several different crystal structures, only the diamond-cubic structure is stable at atmospheric pressure. However, as reported in the Russian literature, a metastable modification of silicon with diamond-hexagonal structure forms during hot indentation of single crystals. Subsequent research activity in the U.S. and Europe confirmed these reports and established the crystallography by means of high-resolution electron microscopy. Researchers at Case Western University determined that the transformation from the diamond-cubic to the diamond-hexagonal structure was of a martensitic nature and developed a model for the observed behavior.

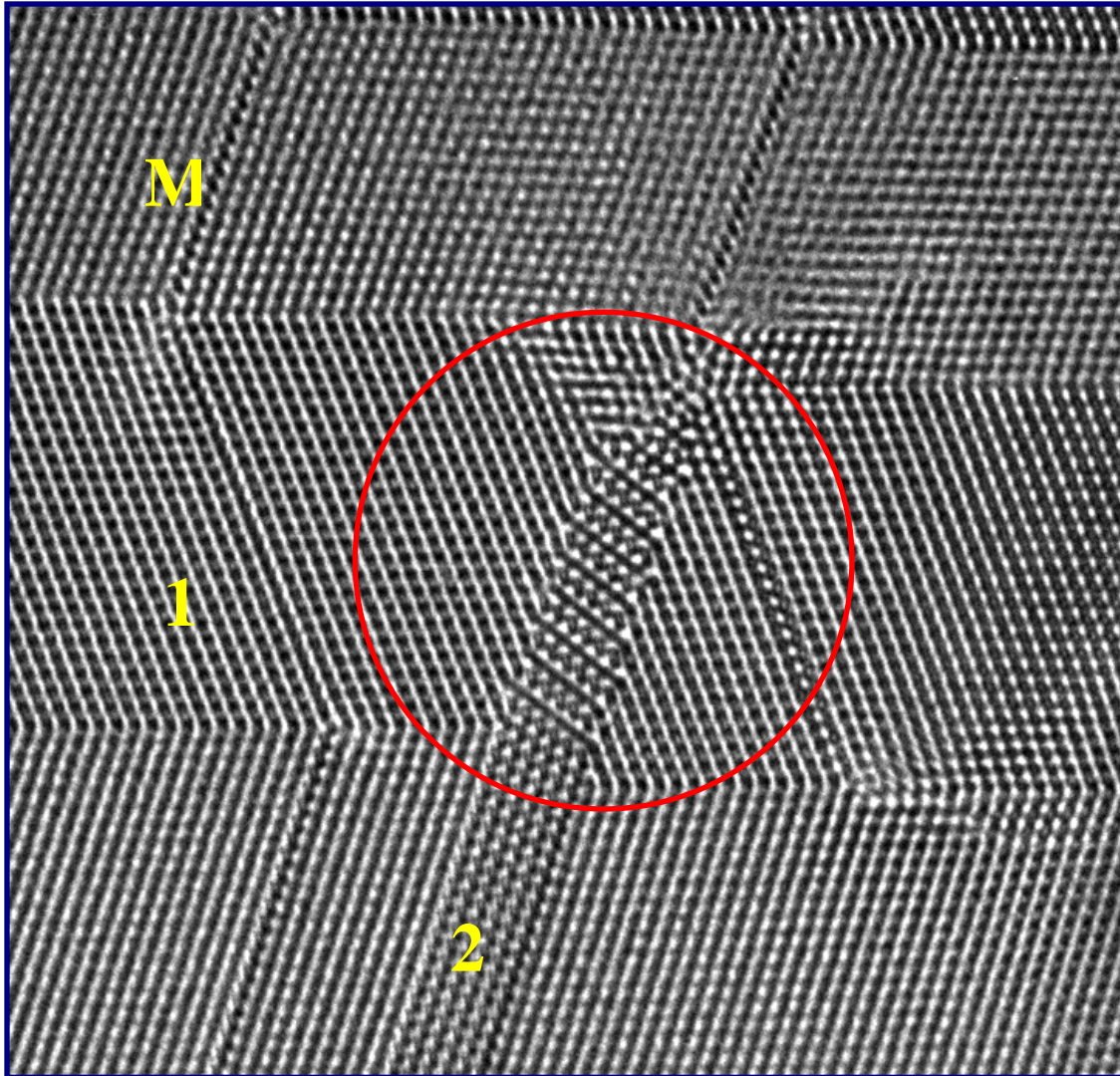
Accomplishment - In this work, the predictions of the model were verified for the first time by direct observation of a nucleus of a hexagonal inclusion by high resolution electron microscopy.

The unique crystallographic features of the hexagonal phase includes a {115} habit plane and an unusual orientation relationship in which close packed planes in the two phases are not parallel. The model for this transformation is based on the hypothesis that the shear strains at intersecting twins can be accommodated by a reverse twinning shear which originates the transformation. A schematic of the model shows how a narrow twin band (1) is intersected by a second twin (2). Strain ac-

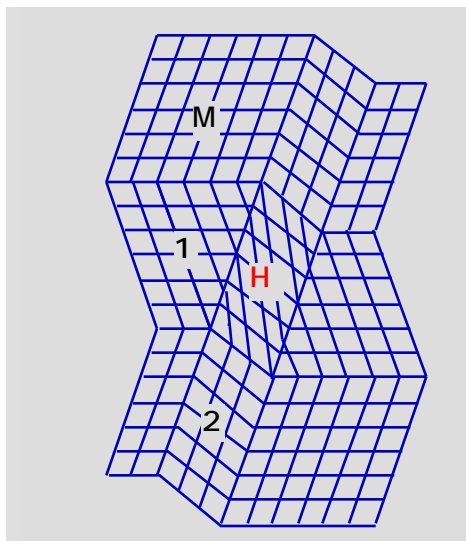
commodation then requires that the crystal structure be changed to hexagonal stacking in the region of intersection. A direct observation of this process was made possible through use of the Atomic Resolution Microscope at NCEM. The high resolution microscope image can be compared directly with the schematic model. The two intersecting twin bands are readily recognized from the different stacking and lattice orientation. As predicted by the model the stacking of close-packed planes in the region of intersection has been changed from the cubic ABC sequence to the hexagonal ABAB sequence. With atomic resolution images of such localized structures it is possible to trace the precise atomic mechanisms of the transformation as well as the exact atomic arrangement at complex interfaces.

An extension of the model predicts an alternative twinning sequence that could lead to much larger bands of hexagonal phase on {115} planes of the matrix. These bands have also been observed and follow the predictions of the crystallographic model in detail, confirming their role in the deformation process during hot indentation.

The model, first confirmed here for silicon, is thought to be of more general applicability to other fcc-based materials of low stacking fault energy.



Above: High resolution micrograph of two intersecting twins in silicon single crystal indented at 400°C. Matrix labeled M, twins labeled 1 and 2, hexagonal phase circled.



Left: Schematic diagrams showing single twin (horizontal) being intersected by a second twin (inclined). Strain accommodation causes the region of intersection to transform to hexagonal stacking (labeled H).

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